Bose-Einstein condensation theory for any integer spin: approach based in noncommutative quantum mechanics

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A Bose-Einstein condensation theory for any integer spin using noncommutative quantum mechanics methods is considered. The effective potential is derived as a multipolar expansion in the non-commutativity parameter (θ) and, at second order in θ, our procedure yields to the standard dipole-dipole interaction with θ^2 playing the role of the strength interaction parameter. The generalized Gross-Pitaevskii equation containing non-local dipolar contributions is found. For ^{52}Cr isotopes $\theta = C_{dd}/4\pi$ becomes $\sim 10^{-11}$ cm and, thus for this value of θ one cannot distinguish interactions coming from non-commutativity or those of dynamical origin.

I. INTRODUCTION

Contrarily to fermions, a set of bosons can occupy a same quantum state as a consequence of the Bose-Einstein statistics. This is a purely quantum effect theorized by S. N. Bose and A. Einstein in 1924. During a very long time many people thought that this effect might be experimentally unrealizable until it was discovered in 1995 [1].

By simplicity, many research papers on Bose-Einstein condensation consider only bosons with spin-0 and an effective contact interactions modeled by a Dirac's Delta function and then, long distance interactions such as the dipole-dipole are not taken into account.

Even though the dipole-dipole contributions are very small in current experiments, recently has been shown, using ^{52}Cr isotopes, that this interaction induces explicit anisotropy effects which can be experimentally measured [2, 3, 4, 5].

Although from microscopic dipole-dipole interactions one can construct effective potentials, still there are so many open questions concerning to the derivation of this effective potential (or pseudopotential) in spite of the intense work in this field [6].

The importance of the dipole-dipole interaction can be seen by considering two bosons with spins $\mathbf{s}_1$ and $\mathbf{s}_2$ interacting at large distances through the potential

$$V = \alpha \left(\frac{\mathbf{s}_1.\mathbf{s}_2 - 3(\mathbf{s}_1.\hat{\mathbf{r}})(\mathbf{s}_2.\hat{\mathbf{r}})}{r^3} \right), \tag{1}$$

where $\mathbf{r}$ is the relative position vector, $\hat{\mathbf{r}} = \mathbf{r}/r$ and α is the interaction strength [7]. The interaction (1) cannot be eliminated even in the dilute gas limit [3] , and therefore (1) should be included in the ultracold gas treatment.

At short distances, considerations above are technically implemented by replacing the two-body interaction simply by a δ-function as the pseudo-potential in the case of contact interactions and, therefore, the effective theory is understood in the Gross-Pitaevskii approach, *i.e* the many-body Hamiltonian becomes

$$H = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla^2 + u(\mathbf{r}) \right) + \sum_{i>j} W(\mathbf{r}_i - \mathbf{r}_j). \tag{2}$$

with $W(\mathbf{r}_i - \mathbf{r}_j) = \gamma\, \delta(\mathbf{r}_i - \mathbf{r}_j)$ where we have set m and $\hbar$ equals 1. By other hand, the wave function in this context becomes the order parameter for the bosonic system.

Next step in this approach is to solve

$$H\ \Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = E\ \Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N), \tag{3}$$

where $\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$ is a symmetric wave function that in the Bose-Einstein phase one can write as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \prod_{i=1}^{N} \psi(\mathbf{r}_i), \tag{4}$$

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where –of course– we have assumed that all the bosons are in the ground state and therefore $\psi(\mathbf{r}_i)$ are the one-particle ground state wave functions. The symmetric product (4) is known as the the Hartree's Ansatz.

Using the Hartree's Ansatz one can write the energy of this many-body system as

$$E_{GP} = \frac{N}{2}\int d^3r \left[\psi^*(\mathbf{r})\left(-\nabla^2 + \omega^2\mathbf{r}^2\right)\psi(\mathbf{r}) + \gamma(N-1)\left(|\psi(\mathbf{r})|^2\right)^2\right], \tag{5}$$

where the one-body potential $u(\mathbf{r})$ has been chosen as a harmonic oscillator one as the trapping to confine the atoms in a ultracold atoms experiment.

Equation (5), by other hand, is a direct consequence of the variational method and the equation of motion obtained by minimizing (5) subject to the normalization condition

$$\int d^3|\psi(\mathbf{r}|^2 = 1, \tag{6}$$

in this context turn out to be

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}\omega^2\mathbf{r}^2 + \gamma(N-1)\,|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = \mu\psi(\mathbf{r}), \tag{7}$$

which is the Gross-Pitaevskii equation and the chemical potential μ was introduced as a Lagrange multiplier that takes into account the condition (6).

In (3), as well as in all the discussion that follows it, except by the symmetry of the wave function, the spin effects are neglected and therefore, in this approximation $\psi(\mathbf{r})$ is a scalar. The purpose of the present paper will be to look at Bose-Einstein condensation theory from the non-commutative quantum mechanics point of view as it was formulated in [8] and derive the Gross-Pitaevskii equation in this context. Additionally we will present the derivation of the pseudopotential in this non-commutative quantum mechanics scenario.

The paper is organized as follows; in Section II we review briefly our previous work on NCQM and magnetic dipole interactions, in Section III we extend the Hartee's approach to many body NCQM and the ideas are applied to Bose-Einstein condensation and generalized Gross-Pitaevskii equations are found. Section V contains our conclusions.

II. NONCOMMUTATIVE QUANTUM MECHANICS AND MAGNETIC DIPOLAR INTERACTIONS

Usually noncommutative quantum mechanics of N particles in three dimensions is a model with a given Hamiltonian $\hat{H}(\hat{p}_i, \hat{x}_j)$, with $\{i,j\} = \{1, 2\ldots, 3N\}$ and deformed canonical commutators (see e.g [9]), *i.e.*

$$[\hat{x}_i, \hat{x}_j] = i\theta_{ij}, \tag{8}$$
$$[\hat{p}_i, \hat{p}_j] = iB_{ij}, \tag{9}$$
$$[\hat{x}_i, \hat{p}_j] = i\delta_{ij}, \tag{10}$$

where θ_{ij} and B_{ij} are constant $3N \times 3N$ matrices.

Although (8)-(10) can be also implemented by using the Moyal product in the phase space, it is more convenient to use commutative variables instead noncommutative ones. Technically this last fact imply to write $\hat{p}$ and $\hat{x}$ according to the rules

$$\hat{x}_i \to \hat{x}_i = x_i + \frac{\theta_{ij}}{2}p_j, \tag{11}$$
$$\hat{p}_i \to \hat{p}_i = p_i + \frac{B_{ij}}{2}x_j, \tag{12}$$

where x_i and p_i are the standard variables satisfying the standard canonical commutators, *i.e.*

$$[x_i, x_j] = 0 = [p_i, p_j],$$
$$[x_i, p_j] = i\delta_{ij},$$

these rules, sometimes known as Bopp's shifts, are the starting point in noncommutative quantum mechanics. We would like to emphasize that the spin properties in the conventional Bopp's shifts does not appears and, therefore, if these effects are incorporated one must to modify these rules.

In reference [8], for the case of one particle in three dimensions, the spin was introduced by positing the algebra

$$\begin{aligned} [\hat{x}_i, \hat{x}_j] &= i\theta^2 \epsilon_{ijk} \hat{S}_k, \\ [\hat{x}_i, \hat{p}_j] &= i\delta_{ij}, \qquad [\hat{p}_i, \hat{p}_j] = 0, \\ [\hat{x}_i, \hat{s}_j] &= i\theta\epsilon_{ijk}\hat{s}_k, \qquad [\hat{s}_i, \hat{s}_j] = i\epsilon_{ijk}\hat{s}_k, \end{aligned} \tag{13}$$

where $\{i, j\} = \{1, 2, 3\}$ and θ is a parameter with dimension of length. Equation (13) is just a deformation of the Heisenberg's algebra similar to the Snyder one [10].

Following [8] one realize that the algebra (13) can be explicitly realized in terms of *commutative* variables by means of the identification

$$\begin{aligned} \hat{x}_i &\to \hat{x}_i = x_i + \theta S_i, \\ \hat{p}_i &\to \hat{p}_i = p_i := -\imath\partial_i, \\ \hat{s}_i &\to \hat{s}_i = s_i, \end{aligned} \tag{14}$$

where x_i and p_i are now canonical operators satisfying the Heisenberg's algebra and S_i are spin matrices. Notice the matricial character of the non-commutative coordinate operators $\hat{x}_i$.

This simple observation implies that any noncommutative quantum mechanical system described by the dynamic equation

$$\imath\partial_t|\psi(t)\rangle = \hat{H}(\hat{p}, \hat{x}, \hat{s})|\psi(t)\rangle = \left[\frac{1}{2}\hat{p}^2 + \hat{V}(\hat{x})\right]|\psi(t)\rangle \tag{15}$$

can equivalently be described by the *commutative* Schrödinger equation

$$\imath\partial_t\psi(\mathbf{x}, t) = H(p_i, x_i + \theta s_i)\,\psi(\mathbf{x}, t)\,, \tag{16}$$

where $\psi(\mathbf{x}, t)$ is a spinor of $2s + 1$-components.

In [8] was discussed that the noncommutative version of the harmonic oscillator whose Hamiltonian is

$$\begin{aligned} H &= -\frac{1}{2}\boldsymbol{\nabla}^2 + \frac{1}{2}\hat{\mathbf{x}}^2, \\ &= -\frac{1}{2}\boldsymbol{\nabla}^2 + \frac{1}{2}\mathbf{x}^2 + \theta\mathbf{x}\,.\,\mathbf{s} + \theta^2\mathbf{s}^2. \end{aligned} \tag{17}$$

The factor $\theta\mathbf{s}^2$ can be absorbed by a renormalization of the ground state energy and, therefore, the new contribution due noncommutativity is the magnetic dipolar interaction $\theta\mathbf{x}\,.\,\mathbf{s}$. Of course if one include many particles effects one should reproduce the dipole-dipole interaction (1), however our main purpose below will be implement effective interactions.

III. APPROACH TO BOSE-EINSTEIN CONDENSATION FOR ANY SPIN

Let us consider N atoms described by the Hamiltonian (2). In order to take into account the spin effects, we use the prescription in (14) in the two-body potential for the non-commutative coordinates $\hat{\mathbf{r}}$ and $\hat{\mathbf{r}}'$ satisfying (13), *i.e.*

$$W(\hat{\mathbf{r}} - \hat{\mathbf{r}}') = W_s(\hat{\mathbf{r}} - \hat{\mathbf{r}}') + W_\ell(\hat{\mathbf{r}} - \hat{\mathbf{r}}'), \tag{18}$$

where W_s and W_ℓ are the contact and large distances contributions respectively.

Let us now write explicitly both potentials up to order θ^2. For the contact interaction we have

$$\begin{aligned} W_s(\hat{\mathbf{r}} - \hat{\mathbf{r}}') &= \gamma\,\delta(\mathbf{r} - \mathbf{r}' + \theta(\mathbf{s} - \mathbf{s}')), \\ &= \gamma\int d^3k e^{i\mathbf{k}\cdot\Delta\mathbf{r}} e^{i\theta\mathbf{k}\cdot\Delta\mathbf{s}}, \\ &= \gamma\,\delta(\mathbf{r} - \mathbf{r}') + \theta\gamma\Delta\mathbf{s}\cdot\nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}') + \frac{\gamma\theta^2}{2}\left(\Delta\mathbf{s}\cdot\nabla_{\mathbf{r}}\right)^2\delta(\mathbf{r} - \mathbf{r}') + \mathcal{O}(\theta^3), \end{aligned} \tag{19}$$

with $\Delta\mathbf{s} = \mathbf{s} - \mathbf{s}'$.

The large distances term turn out to be

$$\begin{aligned} W_\ell(\mathbf{r}-\mathbf{r}') &= \frac{1}{|\mathbf{r}-\mathbf{r}'+\theta(\mathbf{s}-\mathbf{s}')|}, \\ &= \frac{1}{|\Delta\mathbf{r}|}\left[1+\theta\frac{\Delta\mathbf{s}\cdot\Delta\mathbf{r}}{|\Delta\mathbf{r}|^2}-\frac{\theta^2}{2|\Delta\mathbf{r}|^2}\left(\Delta\mathbf{s}^2-3(\Delta\mathbf{s}\cdot\Delta\hat{\mathbf{r}})^2\right)+\mathcal{O}(\theta^3)\right], \end{aligned} \tag{20}$$

where we have defined $\Delta\mathbf{r}=\mathbf{r}-\mathbf{r}'$ and $\Delta\hat{\mathbf{r}}=\Delta\mathbf{r}/|\Delta\mathbf{r}|$.

Since the spin contributions are dominant at large distances, one can neglect the purely coulombian contributions, thus the the potential at large distances becomes

$$W_\ell(\mathbf{r}-\mathbf{r}')\approx\theta\frac{\Delta\mathbf{s}\cdot\Delta\mathbf{r}}{|\Delta\mathbf{r}|^3}-\frac{\theta^2}{2}\frac{\left(\Delta\mathbf{s}^2-3(\Delta\mathbf{s}\cdot\Delta\hat{\mathbf{r}})^2\right)}{|\Delta\mathbf{r}|^3}+\cdots, \tag{21}$$

which contains the dipole and dipole-dipole contributions and so on.

At very large distances, of course there are not contact interactions and the dominant term of the pseudo-potential is (21) which, compared with (1) tells us

$$\alpha=\frac{1}{2}\theta^2. \tag{22}$$

It is interesting to note that the identification (22) is similar to the relationship between NCQM and the Landau's problem, where $\theta=1/B$ corresponds to the magnetic length. This identification becomes exact at the lowest Landau level. In our problem at hand, identification (22) plays a similar role to the non-commutative Landau's one and here θ could be directly extracted from known data. Indeed, following [3] one find that

$$\theta^2=\frac{C_{dd}}{4\pi}=\frac{48a_0\hbar^2}{m}$$

where a_0 is the Bohr's radius and m is the ^{52}Cr isotope mass. We therefore find

$$\theta\sim10^{-11}\mathrm{cm}, \tag{23}$$

which is the analogous of the magnetic field in the Landau problem.

A. Generalized Gross-Pitaevskii equations

Following the Hartree's approach let us consider the derivation of the Gross-Pitaevskii equations; in this approach the functional of energy is

$$E=\frac{<\Psi|\hat{H}|\Psi>}{<\Psi|\Psi>},$$

where $\hat{H}$ is the many body Hamiltonian (2) and is assumed that the N bosons are in the ground state. In this case E becomes[1]

$$\begin{aligned} E &= \int d^3r\left[\psi^*(\mathbf{r})\left(-\frac{1}{2}\nabla^2+\frac{1}{2}\omega^2\left(\mathbf{r}+\theta\mathbf{s}\right)^2\right)\psi(\mathbf{r})+\frac{\gamma}{2}\left(|\psi(\mathbf{r})|^2\right)^2\right] \\ &+ \frac{\gamma\theta}{2}\int d^3r\,d^3r'\psi^*(\mathbf{r})\,\psi^*(\mathbf{r}')\left(\Delta\mathbf{s}\cdot\nabla_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}')+\theta\left(\Delta\mathbf{s}\cdot\nabla_{\mathbf{r}}\right)^2\delta(\mathbf{r}-\mathbf{r}')\right)\psi(\mathbf{r}')\psi(\mathbf{r}) \\ &+ \frac{\theta}{2}\int d^3r\,d^3r'\,\psi^*(\mathbf{r})\,\psi^*(\mathbf{r}')\left(\frac{\Delta\mathbf{s}\cdot\Delta\mathbf{r}}{|\Delta\mathbf{r}|^3}-\frac{\theta}{2}\frac{\left(\Delta\mathbf{s}^2-3(\Delta\mathbf{s}\cdot\Delta\hat{\mathbf{r}})^2\right)}{|\Delta\mathbf{r}|^3}\right)\psi(\mathbf{r}')\psi(\mathbf{r}). \end{aligned} \tag{24}$$

[1] In what follows we have changed the normalization of the wave function as $\psi(\mathbf{r})\to\sqrt{N}\psi(\mathbf{r})$

Using some identities, equation (24) can be written as

$$E = (E_{GP} + E_C + E_D) + \mathcal{O}(\theta^3), \tag{25}$$

The second contribution is

$$E_C = \frac{\gamma\theta}{2}\int d^3r \left[-\nabla n \,\cdot\, \psi^*(\mathbf{r})\mathbf{s}\psi(\mathbf{r}) + (\nabla n\cdot\mathbf{s})\,(\nabla\psi^*\cdot\mathbf{s})\,\psi(\mathbf{r})\right], \tag{26}$$

where $n = |\psi|^2$ is the density of particles.

The energy E_D, by other hand, can be written

$$E_D = \frac{\theta}{2}\int d^3r\, \psi(\mathbf{r})U_{DD}(\mathbf{r})\,\psi(\mathbf{r}), \tag{27}$$

with

$$U_{DD}(\mathbf{r}) = \int d^3r'\psi^*(\mathbf{r}')\left[\frac{\Delta\mathbf{s}\cdot\Delta\mathbf{r}}{|\Delta\mathbf{r}|^3} + \frac{\theta}{2}\frac{\left(\Delta\mathbf{s}^2 - 3(\Delta\mathbf{s}\cdot\Delta\hat{\mathbf{r}})^2\right)}{|\Delta\mathbf{r}|^3}\right]\psi(\mathbf{r}'), \tag{28}$$

which corresponds to the dipole and dipole-dipole contributions.

However, before to minimize (25), one should note that **the depletion** is very small and, therefore, we can leave out all terms containing derivatives of n, thus

$$E_C \approx 0.$$

Finally, using this last fact, we arrive to the following Gross-Pitaevskii equation

$$\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}\omega^2\left(\mathbf{r}+\theta\mathbf{s}\right)^2 + \frac{\gamma}{2}\left|\psi(\mathbf{r})\right|^2 + \frac{\theta}{2}U_{DD}(\mathbf{r})\right]\psi(\mathbf{r}) = \mu\psi(\mathbf{r}), \tag{29}$$

which, except for the dipole term $\frac{\Delta\mathbf{s}\cdot\Delta\mathbf{r}}{|\Delta\mathbf{r}|^3}$, is just the Gross-Pitaevskii equation with the nonlocal interaction discussed in [3].

The non-local equation (29) is complicated to solve. However one could try solve perturbatively this equation by assuming axial symmetry and to adding the non-local term as a perturbation one. In such case at 0-th order one find non-intercating vortices solutions, however the explicit inclusion of U_{DD} could induce drastic changes.

IV. CONCLUSIONS

In this paper we have studied the Bose-Einstein condensates for any integer spin by using non- commutative quantum mechanics as a calculation technique. This procedure induces effective dipole and dipole-dipole interactions which coincide with previous calculations [3, 6]. The comparison with (1) yields to (22) and, therefore, this identification is similar to the relationship between θ and the magnetic length in the Landau problem which is another example where the non-commutative geometry is a useful calculation technique. This last fact follows from the identification between θ and $C_{dd}/4\pi$ which is just the border between non-commutativity effects and dipole-dipole interactions. Only if (22) is holds, then one cannot distinguish interactions coming from non-commutativity or dynamical origin.

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